Development of an Intelligent Data Driven Model of the Binding Energy of Nucleus Using Kernel Ridge Regression Method

*Ajanta Das
Department of Physics, Heritage Institute of Technology

Madhubrata Bhattacharya
Department of Physics, The Heritage College

DebabrataDatta
Department of Information Technology, Heritage Institute of Technology,
Chowbaga Road, Anandapur, Kolkata-700107
India

ABSTRACT. This study explores the use of machine learning techniques, particularly kernel ridge regression (KRR), to refine the estimation of semi-empirical mass formula (SEMF) coefficients, which represent volume energy, surface energy, Coulomb energy, asymmetry energy, and pairing energy. Traditional regression techniques, such as ordinary least square regression (OLSR), are limited by their parametric nature and susceptibility to over fitting, particularly when modeling complex relationships within high-dimensional data. By incorporating a penalty term and kernel functions, KRR mitigates over fitting, reduces variance, and enhances predictive accuracy. Mass number and atomic number data for 109 nuclei were analyzed, with model performance assessed through root mean square error and R^2 values. The findings demonstrate the superior robustness and accuracy of KRR in predicting nuclear binding energy and estimating SEMF coefficients. This work underscores the potential of machine learning in addressing longstanding challenges in nuclear physics, offering a pathway for enhanced theoretical and experimental alignment. Moreover, the incorporation of shell corrections into the traditional Liquid Drop Model (LDM) leads to the development of the Generalized Liquid Drop Model (GLDM). This enhanced approach provides a more comprehensive theoretical framework for understanding nuclear binding energy by accounting for proximity energy and shell effects. It offers improved alignment with experimental observations, effectively explaining phenomena such as magic numbers and nuclear stability trends.

Key words: Semi Empirical Mass Formula, Liquid Drop Model, Kernel Ridge Regression

I. INTRODUCTION.

The semi-empirical mass formula (SEMF) for nuclear binding energy (BE) proposed by Bethe and Weizsäcker is based on Liquid Drop Model (LDM) of N. Bohr and F. Kalckar. For mass number A > 40, SEMF provides BE that is within 1% of the experimentally observed values. It is further to note that nuclear BE is very important not only for nuclear physics [1] but also for a complete understanding of astrophysics [2,3]. Over the past few decades, improvements in experimental facilities have greatly increased the accuracy and scope of nuclear BE measurements. The most recent atomic mass table, AME2016[4] provides with a comprehensive database that provides accurate and precise atomic mass values for isotopes and their nuclear properties which is a key resource in nuclear physics, chemistry and related fields. However, the experiments carried out to generate new data set have some limitations or areas where improvements are necessary. Further the lack of experimental data in the neutron rich or proton rich nuclei region [5-10] and theoretical over extrapolation of nuclear masses of these regions brought into significant uncertainties in their predicted masses. Therefore, development of more refined nuclear models of BE which can be better aligned with experimental results is obligatory at this juncture. Physics design pertaining to the mass formula from theory suggests that nuclear BE is proportional to volume energy and surface energy of the nucleus, coulomb energy, asymmetry energy as well as pairing energy [10] of the nucleus. The proportionalities are adjusted with the relevant constants labelled as coefficients due to volume, surface, coulomb, asymmetry and pairing energy. Researchers have performed experiments and these

*Contact author: ajanta.das@heritageit.edu

coefficients are experimentally determined. All these energies being linearly independent are additive in nature and hence it is possible to formulate a theoretical estimation of these coefficients via regression technique. In this context, several researchers have already attempted ordinary least square regression method to estimate these coefficients. However, ordinary least square regression method being a parametric statistical technique is completely biased on the Gaussian process and hence invites the possibility of over fitting in fitting the related data [11, 12]. Over fitting happens when a model becomes overly intricate and starts to explain the data's random error instead of the correlations between variables. This could lead to deceptive regression coefficients, R-squared values, and p-values, which would make it difficult to draw valid conclusions from the data. Details of ordinary least square regression method (OLSRM) can be found in [12], wherein we look for minimizing the square of the error between experimental value and theoretical formulation of binding energy of the nuclei. The issue of over fitting data in OSLRM further invites a substantial uncertainty in the estimated value of the coefficients and is solved by applying machine learning oriented regression method such as ridge regression. Ridge regression reduces uncertainty by lowering the variance of the estimates and shrinking the regression coefficients towards zero by including a penalty term in the regression equation. By lessening the influence of noisy or unnecessary predictors in the model, this helps to avoid overfitting. Ridge regression can assist to find the most significant predictors and increase the model's accuracy, which is especially helpful when working with high-dimensional data, when there are many more predictors than observations. Several areas of nuclear physics have effectively used machine learning techniques [13-15]. Since theoretical formulation of binding energy of the nucleus possess nonlinear boundary of the data due to the presence of different energy terms, we need to look at suitable kernel for ridge regression and hence we have adopted kernel ridge regression (KRR) method in fitting the experimental values of binding energy data. KRR is a method for machine learning that uses a kernel function to predict a target variable by fitting a ridge regression model. It helps in achieving accurate predictions by removing bias and improving the performance of the model. With a view to estimate the coefficients of semi-empirical mass formula by machine learning oriented regression method and also to handle the over fitting issue in fitting the experimental nuclear BE values, we have implemented both OLSRM model as well as KRR method. A and Z values of 109 nuclei are used as input to our regression model and the model performance is evaluated by estimating rms error and goodness of fit value, R^2.

I.I. RESEARCH OBJECTIVES

Our objective is to promote the machine learning oriented regression model of semi-empirical mass formula by kernel ridge regression method and also to compare the performance of KRR models and traditional statistical methods in predicting binding energies of atomic nuclei. The study also aims to evaluate robustness, and interpretability of both approaches to evaluate the coefficients of the SEMF for nuclear BE.

I.II. RELATED WORK

Recently, the accuracy of nuclear models has been increased through the use of machine learning approaches such as the Bayesian neural network (BNN) [16–19], radial basis function (RBF) [20–22], and KRR approach [23]. However, the mass predictions generated by the RBF and BNN techniques diverge significantly for nuclei that are positioned outside of the range of known masses [24].Whereas KRR approach determines the extrapolation distance limit to avoid the potential degradation of nuclear mass estimations at longer extrapolation distances. Wu et. al. uses KRR approach with Gaussian kernel to enhance the predictions of nuclear mass[23]. The authors expanded the KRR technique in a different study to include the odd-even effects in nuclear mass prediction [25]. Huang et. al. applied KRR in forecasting the reaction cross sections of neutron capture [26] and successfully reduced the rms deviation in experimental result and predicted value from 69.8% to 35.4%.Literature review also provides an update of implementing KRR approach of data fitting for prediction of nuclear mass by using kernel functions like Laplacian, Gaussian, Matern, Multiquadric, Cauchy, inverse Multiquadric, power and inverse power function recently been used for [27]. Notably, the Gaussian kernel approach has been observed to outperform other kernel functions in this context.Wu and Pan recently created the anisotropic kernel ridge regression [28] for prediction of nuclear mass by using the kernel ridge regression (KRR) technique and adding the anisotropic kernel function without requiring the addition of a new training input or weight parameter. Predictions for interpolation and extrapolation have been improved with the usage of a double two-dimensional Gaussian kernel. In this context, it is to be noted that no researchers have

*Contact author: ajanta.das@heritageit.edu

applied kernel ridge regression technique to fit the data pertaining to binding energy values of the nuclei for estimating the coefficients of SEMF.

The paper is delivered as follows: section II presents the physics of the binding energy of the nuclei and its efficacy to present the generalized liquid drop model (a new concept), section III describes the mathematical method of ordinary least square regression towards fitting of binding energy formulation as well as the computational details of Kernel Ridge Regression; Section IV provides the results of our fitting and claims the success of machine learning oriented regression approach in bringing a conceptual framework of generalized liquid drop model. Finally, section V concludes by highlighting key findings and discussing potential directions for future research in this field.

II. PHYSICS OF BINDING ENERGY OF NUCLEI

The analogy of a nucleus with a liquid drop stems from the observations on the systematic of nuclear BE which is defined as the energy needed to hold the nucleons together, forming the nucleus.The nuclear BE having Z protons and N neutrons is given by

$$BE(Z,N) = [Z M_p + N M_n - M(Z,N)]c^2 \quad (1)$$

where M_p and M_n are the proton mass and neutron mass respectively. This is a spent energy and is therefore negative. To describe the general characteristics of nuclides, a variety of models have been put forth. One of the earliest and simplest models was the LDM, introduced by Weizsäcker and later refined by Bohr and Wheeler. The LDM was highly effective in predicting binding energies of nuclei. Besides, this was the only model which explained the phenomenon of fission. This model is based on three fundamental principles such as nuclides can be approximated as droplets of incompressible liquid, uniform nuclear forces acting on all nucleons, and the saturation characteristic of nuclear forces. From these assumptions, SEMF, also known as the Bethe-Weizsäcker formula [29], was constructed empirically and the same to express nuclear BE can be mathematically expressed as,

$$B_E = a_v A - a_s A^{\frac{2}{3}} - a_c Z(Z-1)A^{-\frac{1}{3}} - a_a (A-2Z)^2 A^{-1} + \delta(N,Z) \quad (2)$$

where, consecutive terms in the right side of Eqn. (2) represents the terms corresponding to the nucleon cohesion, surface tension, proton repulsion, neutron-proton ratio and even odd effects respectively. The constants of expression as presented in Eqn. (2) are required to best fit the experimental data. The last term in Eqn. (2) that is, $\delta(N,Z)$ is due to odd-even effects of nuclei and is known as pairing energy term. It is imperative to discuss about the pairing energy term in the process of data fitting of binding energy nuclei. Physics of the binding energy can be focused towards the pairing energy and is presented in sub section II.I.

II.I. PAIRING ENERGY

The even-odd nature of the nucleus determines the small but consistent variations in the overall binding energies, which results in a term known as the Pairing Energy, represented by $\delta(N,Z) = E_p$. When feasible, nucleons of the same kind exist in pairs because they prefer to occupy the same orbital. In chemistry, Hund's Rule states that electrons prefer distinct orbits; this is the exact opposite. When electrons in atoms are as far apart as feasible, the electromagnetic repulsive force between them is reduced, favouring various orbits. The nuclear interaction between nucleons, however, is attracting. In order to optimize the attraction, protons and neutrons team up and share the same orbital whenever Z or N is even. When A is even, the options with (Z, N) are odd- odd (o-o) or even- even (e-e), whereas, for odd A, even-odd (e-o) or odd-even (o-e) are the options. Table I lists the stable isotopes of each kind.

TABLE I. of stable isotopes as a function of odd and even Z, N

	(e-e)	(e-o)	(o-e)	(o-o)
No. of isotopes	157	55	50	4

The binding energy formula is expanded to include the fifth term (Eqn. (2)) in order to account for the pairing energy and we write it as $E_p = a_p \gamma / A^{1/2}$, where γ = +1 (e-e), 0 (o-e and e-o) and -1 (o-o) respectively. The present research is focused to fit the coefficients of Eqn. (2) using ordinary least square method and machine learning method. This is also to understand whether machine

*Contact author: ajanta.das@heritageit.edu

learning approach is suitable for the experimental data fitting of nuclear BE. Thrust area of the present research is also seeking to formulate a generalized liquid drop model and the same is described in sub section II.II.

II.II. GENERALISED LIQUID DROP MODEL

Recent fusion physics studies have shown that to offer accurate fusion cross sections, the pure Coulomb barrier image is insufficient. The impact of the nuclear forces in the fissure where the neck is formed or in the space between the incoming close nuclei must be considered while adding a proximity energy factor. By combining the proximity energy and a quasi-molecular form sequence, this automatically increases the possibility of a Generalized Liquid Drop Model (GLDM) that can depict the fusion process and proximity energy optimization.

This study allows one to reproduce the fission data in the deformation valley. The computations reveal an effective degeneracy in the energy levels of compact and necked configurations, which is mitigated by incorporating nuclear proximity effects. On the other hand, extended shapes have energy determined by the liquid drop model without considering proximity effects. The consistency with the fission and fusion data has ultimately resulted in the exploration of the entrance and departure pathways of superheavy nuclei, as well as the alpha and cluster radioactivity. The sum of the energy from the Rotational LDM and the nuclear proximity energy for an arbitrary deformed nucleus is the macroscopic total energy [30].

Assuming the conservation of volume and density, we can write the macroscopic total energy as

$$E = E_V + E_S + E_C + \frac{l(l+1)}{2I}, \quad (3)$$

Note: Planck's constant h is assumed as 1 for convenience of computation. The mathematical formulae of E_V, E_S, E_C without derivation can be written as

$$E_V = -a_V\left(1 - k_V([(N-Z)/A]^2)\right)A \quad (4)$$

$$E_S = a_S\left(1 - k_S\left(\left[\frac{N-Z}{A}\right]^2\right)\right)A^{\frac{2}{3}}\left(\frac{S}{4\pi R_0^2}\right) \quad (5)$$

$$E_C = 0.6e^2\left(Z^2/R_0\right)0.5\int\left(\frac{V(\theta)}{V_0}\right)\left(\frac{R(\theta)}{R_0}\right)^3.\sin(\theta)\,d \quad (6)$$

Eqn.s (4), (5), and (6) can be changed upon separation of the two colliding nuclei. With the altered expression, at the contact location, there is a discontinuity of a few MeV. When the $\frac{Z}{A}$ ratios differ greatly. Since this discontinuity results from the gradual rearrangement of the nuclear matter, it has been removed in a linear fashion from the point of contact to the sphere. The surface energy only considers the effect of surface tension forces in a half space and excludes the inputs from the gap between entering nuclei or nascent fragments or the attractive nuclear contacts between the surfaces in the neck. When crevices emerge in the path of deformation, these extra surface effects are taken into consideration by using the energy term E_N for nuclear proximity. With an attenuation factor, the shell corrections as described in the Droplet Model [30] can be expressed as

$$E_{shell} = E_{sphere}^{shell}(1 - 2.6\alpha^2)\exp(-\alpha^2) \quad (7)$$

Where, $\alpha a = \delta R =$ distortion. Shell adjustments in this situation are dependent on the nucleus's deformation, and by employing this method, they only affect the compound nucleus close to its ground state rather than at the saddle-point, where they are expected to be approximately 1 MeV or less. Therefore, BE formulation pathway is searched for introducing the shell correction and this mode of shell correction in the LDM when introduced we define that model as GLDM which is one of the research components of the present research. Let us now define how this shell correction looks like and whether binding energy formulation can help or not. Magic nuclei are not explained by the traditional liquid drop hypothesis. Experimental data show that nuclei exhibit greater stability at the magic values, which create shell closure for Z and N.

Compared to their neighbouring nuclei, the magic nuclei are more stable. Depending on the energy difference between Z and N, we can have

*Contact author: ajanta.das@heritageit.edu

$$S_p = B(A, Z) - B(A-1, Z-1) \quad (8)$$

$$S_n = B(A, Z) - B(A-1, N-1) \quad (9)$$

Therefore,

$$S_p - S_n = B(A-1, N-1) - B(A-1, Z-1) = -a_c(2Z-1)(A-1)^{1/3} + a_a\frac{(A-2Z)}{(A-1)} \quad (10)$$

For a stable nuclei,

$$Z \cong A/2\left(1 - \frac{a_c}{a_a}A^{2/3}\right), \text{ so,}$$

$$S_p - S_n = \frac{a_c}{A}\frac{a_c}{a_a}A^{7/3} = \frac{a_c^2}{a_a}A^{4/3} \quad (11)$$

The term $\frac{a_c^2}{a_a}$ is termed as shell correction and is denoted as a_{shell}. Therefore, best estimate under uncertainty presence in the measurement necessitates the accuracy of the shell correction by which using liquid drop model one can easily define magic numbers which is an innovative concept in present day's study of nuclear binding energy. Introduction of the shell correction in the conventional binding energy formulation results a new binding energy formula which can be formulated qualitatively as

Modified Binding Energy = Old Binding Energy + shell correction. This modified binding energy is termed as GLDM.

III. MATHEMATICAL METHODS OF DATA FITTING

To fit the experimental values of the nuclei's binding energy, two approaches have been tried.
In the first case, we have merely illustrated the application of the standard least squares approach, wherein the coefficients of the said formulation are estimated in terms of matrix method such as Ax = B. Assuming the chance of overfitting in the previous case, we have attempted next a machine learning technique using Kernel Ridge Regression (KRR), where independent variables are replaced by suitable kernel. Performance of both the approaches have compared with respect to the estimation of root mean square value and the goodness of fit parameter. Sub section III.I and III.II presents the mathematics behind these two methods.

III.I. THE LEAST SQUARES METHOD

LSM is a commonly used technique for data fitting, as highlighted in [13]. Finding approximate solutions to over-determined systems—systems with more equations than unknowns—is a common practice in regression analysis. When determining constants in theoretical formulas based on actual data, this approach works especially well. The term "least squares" refers to minimizing the total sum of the squared differences (errors) between observed and predicted values across all equations in the system.
The LSM is most widely applied in data fitting. Subject to the linearity of the residuals with respect to the unknown parameters, least square (LS) problems can be classified as either linear (ordinary) or non-linear. Linear LSs problems, which are prevalent in statistical regression, have straightforward closed-form solutions. Non-linear least squares problems, on the other hand, are typically addressed using iterative methods. In these methods, the system is approximated as linear at each step, ensuring that the core calculations remain similar for both types of problems. We have the SEMF as

$$BE_{Theo} = a_v A + a_s A^{2/3} + a_c \frac{Z(Z-1)}{A^{1/3}} + a_a \frac{((A-2Z)^2}{A} \quad (12)$$

Where BE_{Theo} represents the semi empirical nuclear binding energy and a_v, a_s, a_c and a_a denote the coefficients of volume, surface, coulomb and asymmetry term respectively. Our aim is to determine the coefficients from existing binding energy data (experimental) for several nuclei. Applying LSM we have our error function as

*Contact author: ajanta.das@heritageit.edu

$$S = \sum_i \left[\left(BE\right)_{i,Expt} - \left(BE\right)_{i,Theo} \right]^2$$

$$= \sum_i \left[\left(BE\right)_{i,Expt} - \left\{ a_v A_i + a_s A_i^{2/3} + a_c \frac{Z_i (Z_i - 1)}{A_i^{1/3}} + a_a \frac{(A_i - 2Z_i)^2}{A_i} \right\} \right]^2 \quad (13)$$

To minimize the error in eqn. (13), we have

$$\frac{\partial S}{\partial a_v} = -2 \sum_i A_i \left[\left(BE\right)_i - \left\{ a_v A_i + a_s A_i^{2/3} + a_c \frac{Z_i (Z_i - 1)}{A_i^{1/3}} + a_a \frac{(A_i - 2Z_i)^2}{A_i} \right\} \right]$$

$$\frac{\partial S}{\partial a_s} = 2 \sum_i A_i^{2/3} \left[\left(BE\right)_i - \left\{ a_v A_i + a_s A_i^{2/3} + a_c \frac{Z_i (Z_i - 1)}{A_i^{1/3}} + a_a \frac{(A_i - 2Z_i)^2}{A_i} \right\} \right]$$

$$\frac{\partial S}{\partial a_c} = 2 \sum_i \frac{Z_i (Z_i - 1)}{A_i^{1/3}} \left[\left(BE\right)_i - \left\{ a_v A_i + a_s A_i^{2/3} + a_c \frac{Z_i (Z_i - 1)}{A_i^{1/3}} + a_a \frac{(A_i - 2Z_i)^2}{A_i} \right\} \right]$$

$$\frac{\partial S}{\partial a_a} = 2 \sum_i \frac{(A_i - 2Z_i)^2}{A_i} \left[\left(BE\right)_i - \left\{ a_v A_i + a_s A_i^{2/3} + a_c \frac{Z_i (Z_i - 1)}{A_i^{1/3}} + a_a \frac{(A_i - 2Z_i)^2}{A_i} \right\} \right] \quad (14)$$

Eqn. (14) reduces to

$$\begin{pmatrix} X_{11} & X_{12} & X_{13} & X_{14} \\ X_{21} & X_{22} & X_{23} & X_{24} \\ X_{31} & X_{32} & X_{33} & X_{34} \\ X_{41} & X_{42} & X_{43} & X_{44} \end{pmatrix} \begin{pmatrix} a_v \\ a_s \\ a_c \\ a_a \end{pmatrix} = \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{pmatrix} \quad (15)$$

Where,

$$X_{11} = \sum_i A_i^2,$$

$$X_{12} = X_{21} = -\sum_i A_i^{5/3},$$

$$X_{13} = X_{31} = -\sum_i Z_i (Z_i - 1) A_i^{2/3},$$

$$X_{14} = X_{41} = -\sum_i (A_i - 2Z_i)^2,$$

$$X_{22} = \sum_i A_i^{4/3},$$

$$X_{23} = X_{32} = \sum_i Z_i (Z_i - 1) A_i^{1/3},$$

$$X_{24} = X_{42} = \sum_i (A_i - 2Z_i)^2 / A_i^{1/3},$$

$$X_{33} = \sum_i Z_i^2 (Z_i - 1)^2 / A_i^{2/3},$$

$$X_{34} = X_{43} = \sum_i Z_i (Z_i - 1)(A_i - 2Z_i)^2 / A_i^{4/3},$$

$$X_{44} = \sum_i (A_i - 2Z_i)^4 / A_i^2. \quad (16)$$

And

$$Y_1 = \sum_i A_i \left(BE\right)_{i,Expt},$$

$$Y_2 = -\sum_i A_i^{\frac{2}{3}} \left(BE\right)_{i,Expt},$$

$$Y_3 = -\sum_i \frac{Z_i (Z_i - 1)}{Ai^{\frac{1}{3}}} \left(BE\right)_{i,Expt}$$

$$Y_4 = -\sum_i \frac{(A_i - 2Z_i)^2}{A_i} \left(BE\right)_{i,Expt} . \quad (17)$$

From Eqn. (15), we can write the regression equation:

*Contact author: ajanta.das@heritageit.edu

$$\begin{pmatrix} a_{\nu} \\ a_{s} \\ a_{c} \\ a_{a} \end{pmatrix} = \begin{pmatrix} X_{11} & X_{12} & X_{13} & X_{14} \\ X_{21} & X_{22} & X_{23} & X_{24} \\ X_{31} & X_{32} & X_{33} & X_{34} \\ X_{41} & X_{42} & X_{43} & X_{44} \end{pmatrix}^{-1} \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{pmatrix} \quad (18)$$

III.II. MATHEMATICAL FORMULATION OF KERNEL RIDGE REGRESSION

Kernel Ridge Regression (KRR), a dependable machine learning, has been effectively utilised to predict to nuclear mass [23]. In this research, the coefficients of binding energy are evaluated using KRR with linear kernel. In KRR, the complexity of the learned model is controlled by the use of kernels to translate data into a higher-dimensional feature space where the link between input and target can be approximated linearly. The Kernel function is written as

$$S(x_i) = \sum_{j=1}^{n} K(x_i, x_j)\,\alpha_j \quad (19)$$

Where α_j represents the weight parameters, the kernel function $K(x_i, x_j)$ is used to quantify the correlations between nuclei. In order to calculate the parameters α_j, the cost function was minimized and specified as

$$C(\alpha) = \sum_{j=1}^{n} [S(x_i) - y(x_i)]^2 + \lambda \|\alpha\|^2 \quad (20)$$

Where, $= (\alpha_1, \ldots\ldots \alpha_n)$. To reduce the chance of over-fitting, the second term in equation (20) penalizes high weights. The severity of the penalty is determined by the hyper-parameter λ. Minimizing the cost function will deliver

$$\alpha = (K + \lambda I)^{-1} y \quad (21)$$

Where, K and I denote the kernel matrix and the identity matrix, respectively. The linear kernel is defined as

$$K = X^T X = \begin{pmatrix} x_1^T x_1 & x_1^T x_2 & x_1^T x_3 & x_1^T x \\ x_2^T x_1 & x_2^T x_2 & x_2^T x_3 & x_2^T x \\ x_3^T x_1 & x_3^T x_2 & x_3^T x_3 & x_3^T x \\ x_4^T x_1 & x_4^T x_2 & x_4^T x_3 & x_4^T x \end{pmatrix} \quad (22)$$

Where we have rewritten Eqn. (12) as

$$\varphi(X) = a_{\nu} x_1 + a_{s} x_2 + a_{c} x_3 + a_{a} x_4 \quad (23)$$

One significant benefit of using kernels is that we can operate directly with K without explicitly specifying $\varphi(x)$.

IV. RESULTS AND DISCUSSION

Table II presents the input data used for this calculation. Nuclear BE per nucleon has been plotted (FIG 1) against the mass number using the experimental binding energy.

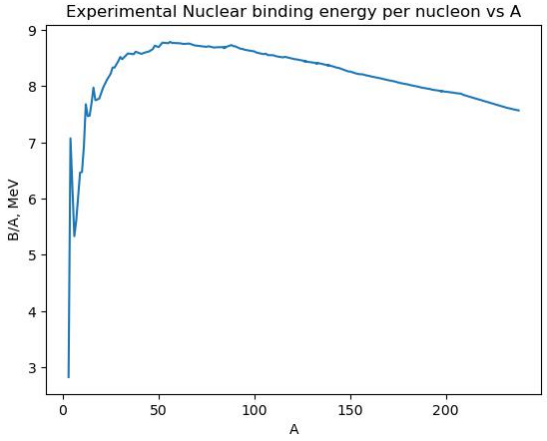

FIG 1. Nuclear binding energy per nucleon vs mass number graph using the experimental data

*Contact author: ajanta.das@heritageit.edu

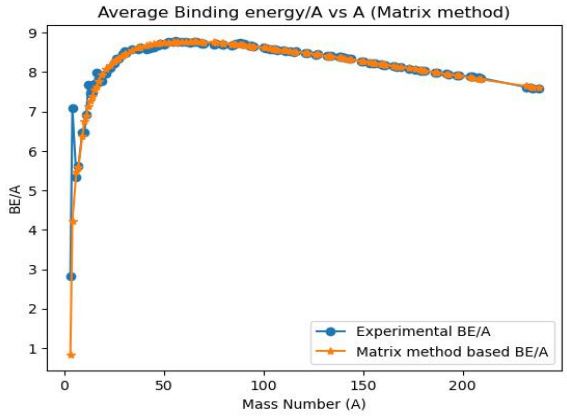

FIG 2. Nuclear binding energy graphs obtained from LSM and experimental data

The data matrix needed for LSM has been formed (Eqn. 16) with the help of nuclear binding energy data displayed in Table 2. The volume, surface, coulomb and asymmetry coefficients obtained through LSM are as follows:

$a_v = 15.75$ MeV, $a_s = 17.94$ MeV, $a_c = 0.72$ MeV,
$a_a = 22.25$MeV.

LSM predicted binding energies are further obtained using these calculated coefficients, and an average BE/A vs. A graph has been plotted (Fig 2.)). The graph mentioned above closely aligned with the experimental one, demonstrating good accuracy.

The regression model demonstrated high predictive accuracy for nuclear binding energies when evaluated against experimental data. By minimizing the cost function the KRR model effectivelystrikes a compromise between model complexity and variance, controlled by the hyper-parameter λ. The use of the kernel matrix K as defined in Eqn. (22) efficiently captures the linear relationships in the high-dimensional feature space, contributing to the accuracy of the binding energy coefficients. The coefficients a_v, a_s, a_c and a_a defined in Eqn. (23), provide a quantitative measure of the contributions from volume, surface, Coulomb, and asymmetry effects, respectively, to the BE. The linear kernel ensures that these contributions are evaluated based on intrinsic correlations within the nuclear data, allowing for a straightforward interpretation. Here it is worth mentioning that the authors tried other kernel functions (like Gaussian, quadratic etc.) but for all other functions the R^2 values were poor. The values of the coefficients obtained through the KRR approach are as follows:

$a_v = 15.75$ MeV, $a_s = 17.93$ MeV, $a_c = 0.72$ MeV,
$a_a = 22.19$MeV.

Furthermore, KRR predicted binding energies are obtained and has been plotted against A (FIG 3.) which shows a good fit with the experimental plotting. The RMSE value for KRR predicted binding energy is obtained as 0.3419. The R squared value defined as $R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$, where SS_{res} denotes the sum of residuals squired and SS_{tot} is the total sum of squares. In the present work the R^2 value is obtained as 0.81 which shows that the model explains 81% of the variance in the dependent variable, indicating a good fit.

In the next part of the work authors calculated $S_p - S_n$ values to get the shell correction term $a_{shell} = \frac{a_c^2}{a_a} = -0.0105$ as the correct ion coefficient. Including a_{shell}, the modified binding energy has been calculated and FIG 4. shows the corresponding plot along with the experimental and KRR predicted values.

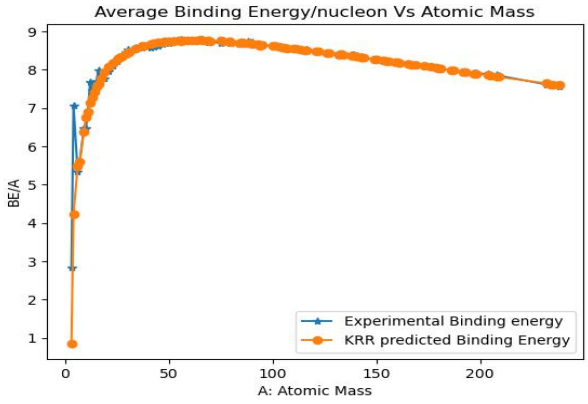

FIG 3. Nuclear binding energy graphs obtained from KRR and experimental data

*Contact author: ajanta.das@heritageit.edu

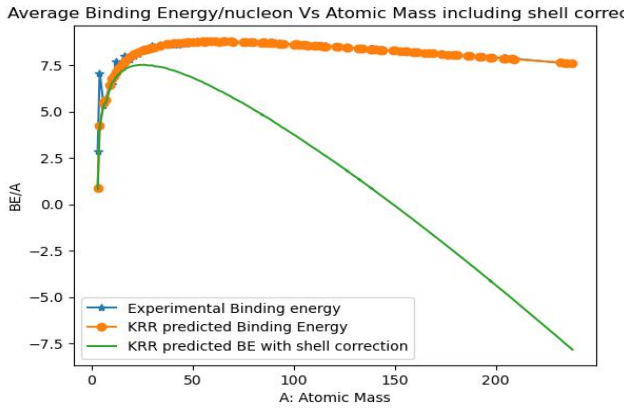

FIG 4. Nuclear binding energy graphs for experimental, KRR and shell correction

TABLE II. Nuclear binding energy data

Nucleus	Z	A	BE/A (MeV)	Nucleus	Z	A	BE/A (MeV)	Nucleus	Z	A	BE/A (MeV)
H	1	3	2.827	Ni	28	61	8.765	Ba	56	134	8.400
He	2	4	7.074	Cu	29	63	8.752	La	57	138	8.375
Li	3	6	5.332	Cu	29	65	8.757	La	57	139	8.378
Li	3	7	5.606	zn	30	66	8.759	Ce	58	138	8.377
Be	4	9	6.463	Ga	31	69	8.725	Pr	59	141	8.354
B	5	10	6.475	Ge	32	70	8.722	Nd	60	143	8.331
B	5	11	6.928	As	33	75	8.701	Nd	60	144	8.327
C	6	12	7.680	Se	34	76	8.711	Sm	62	149	8.264
C	6	13	7.470	Br	35	79	8.688	Sm	62	150	8.262
N	7	14	7.476	Kr	36	80	8.693	Eu	63	153	8.229
N	7	15	7.699	Rb	37	85	8.697	Gd	64	155	8.213
O	8	16	7.976	Sr	38	84	8.677	Gd	64	156	8.215
O	8	17	7.751	Sr	38	86	8.708	Tb	65	159	8.189
F	9	19	7.779	Sr	38	88	8.733	Dy	66	160	8.184
Ne	10	21	7.972	Y	39	89	8.714	Dy	66	161	8.173
Na	11	23	8.111	Zr	40	90	8.710	Ho	67	165	8.147
Mg	12	25	8.224	Nb	41	93	8.664	Er	68	167	8.132
Mg	12	26	8.334	Mo	42	94	8.662	Tm	69	169	8.115
Al	13	27	8.332	Mo	42	95	8.649	Yb	70	173	8.087
Si	14	29	8.449	Ru	44	100	8.620	Lu	71	176	8.059
Si	14	30	8.521	Ru	44	101	8.601	Hf	72	179	8.038
P	15	31	8.481	Rh	45	103	8.584	Hf	72	180	8.035
S	16	34	8.584	Pd	46	105	8.570	Ta	73	181	8.023
Cl	17	37	8.570	Pd	46	106	8.580	W	74	186	7.989
Ar	18	38	8.614	Ag	47	107	8.554	Re	75	187	7.978
Kr	19	41	8.576	Cd	48	110	8.551	Os	76	192	7.949
Ca	20	43	8.600	Cd	48	111	8.537	Ir	77	193	7.938

*Contact author: ajanta.das@heritageit.edu

SC	21	45	8.619	In	49	113	8.523	Pt	78	198	7.914
Ti	22	47	8.661	Sn	50	115	8.514	Au	79	197	7.916
Ti	22	48	8.723	Sn	50	116	8.523	Hg	80	204	7.886
V	23	50	8.696	Sb	51	121	8.482	TI	81	205	7.878
Cr	24	52	8.776	Te	52	122	8.478	Pb	82	208	7.867
Mn	25	55	8.765	I	53	127	8.445	Bi	83	209	7.848
Fe	26	56	8.790	Xe	54	126	8.444	Th	90	232	7.6153
Fe	26	57	8.770	Cs	55	133	8.410	U	92	234	7.601
Co	27	59	8.768	Ba	56	132	8.410	U	92	235	7.591

V. CONCLUSIONS

Machine learning techniques, particularly KRR, provide a robust framework for modelling complex phenomena like nuclear binding energy by improving its predictive accuracy when compared to traditional methods like the Ordinary Least Squares Regression Method (OLSRM). While OLSRM provides a straightforward parametric method for fitting nuclear binding energy data, it is prone to overfitting and higher prediction errors. KRR, with its penalty term and kernel function, overcomes these limitations and demonstrates superior performance metrics such as reduced root mean square error and improved goodness of fit (R^2 values).This is evident from the close alignment of the predicted binding energy values with experimental data. Additionally, the linear kernel used in KRR simplifies interpretability, enabling clearer insights into the relationship between input variables (mass and atomic number) and binding energy. The inclusion of shell corrections in the traditional LDM further leads to the formulation of the GLDM. This approach improves the theoretical understanding of nuclear binding energy, incorporating proximity energy and shell corrections to better explain experimental observations, including magic numbers and stability trends. The success of the KRR approach in estimating SEMF coefficients opens new avenues for the development of advanced nuclear binding energy models. The proposed GLDM framework, combined with machine learning techniques, offers a promising path for future studies in nuclear structure, fusion physics, and astrophysical nucleosynthesis. However, there remains potential for a further generalized model [17-18] that integrates nuclear deformation terms to account for non-spherical shapes, particularly relevant for heavy nuclei. This could be complemented by a shell effect term to integrate quantum mechanical corrections (e.g., shell model inputs), explaining magic numbers more effectively. A thermodynamic term would be essential to predict nuclear behavior under astrophysical conditions. Furthermore, a blend of collective (macroscopic) and individual (microscopic) nucleon behaviors could be incorporated to improve the model's accuracy. Such a generalized nuclear model would offer enhanced predictive power, accurately forecasting phenomena like fission barriers, decay rates, and energy spectra. This improved understanding would be invaluable for simulating astrophysical processes, such as nucleosynthesis, neutron star crust formation, and supernova explosions, shedding light on the elemental evolution of the universe. In nuclear reactions, this model would refine predictions of fusion and fission energy yields, supporting experimental research and optimizing reactor designs. Additionally, it could be applied to exotic nuclei, including unstable, neutron-rich, and proton-rich varieties near the edges of nuclear stability, providing valuable insights into their properties and expanding our understanding of fundamental nuclear physics. Therefore, integrating macroscopic nuclear fluid properties with microscopic quantum effects, a generalized liquid drop model could serve as a robust framework for addressing the challenges in nuclear physics.

VII. DECLARATIONS

A. Authors' Contributions

Each author had participated sufficiently in the work to take responsibility for appropriate portions of the content. All authors read and approved the final manuscript.

*Contact author: ajanta.das@heritageit.edu

B. Competing Interests

The authors declare that they had no competing interests.

C. Availability of Data

The data is available in Evaluated Nuclear Data File (ENDF).

D. Funding

Not applicable

[1] D. Lunney, J. M. Pearson, and C. Thibault, Rev. Mod. Phys. **75**, 1021 (2003).

[2] E. M. Burbidge, G. R. Burbidge, W. A. Fowler, and F. Hoyl, Rev Mod Phys **29**, 547 (1957).

[3] M. R. Mumpower, R. Surman, G. C. McLaughlin, A. Aprahamian, Prog. Part. Nucl. Phys. **86** (2016).

[4] M. Wang, G. Audi, F. G. Kondev, W. Huang, S. Naimi, and X. Xu, Chinese Physics C **41**, 030003 (2017)

[5] P. Moller, A. Sierk, T. Ichikawa and H. Sagawa, Atom Data and Nucl. Data Tables **109**, 1-204 (2016).

[6] N. Wang, M. Liu, X. Wu and J. Meng, Phys. Lett. B **734**, 215-9 (2014).

[7] S. Goriely, N. Chamel, J. M. Pearson, Phys. Rev. C **88,** 024308 (2013).

[8] J. Duflo, A. Zuker, Phys. Rev. C **52**, R23-7 (1995).

[9] J. Pearson, R. Nayak, S. Goriely, Phys. Lett. B **387**, 455-9 (1996).

[10] H. Koura, T. Tachibana, M. Uno, M. Yamada, Prog. Theor. Phys **113**, 305-25 (2005).

[11] G. Carleo, I. Cirac, K. Crammer, I. DaudetI, M. Schuld, N. Tishby et al. Rev. Mod. Phys **91**, 045002 (2019).

[12] A. Boehnlein, M. Diefenthaler, N. Sato, M. Schram, V. Ziegler, C. Fanelli, et al. Rev. Mod. Phys **94**, 031003(2022).

[13] Stephen M. Stigler, The history of statistics: The measurement of uncertainty before 1990. Harvard University Press, (1986)

[14] James E. Martin, Physics for radiation protection. John Wiley & Sons, (2013).

[15] M. A. V. Mirazaei, M. Mohsen, and A. M. Bagher, Nuclear Science **2**, 11 (2017).

[16] R. Utama, J. Piekarewicz, H. B. Prosper, Phys. Rev. C **93**, 014311 (2016).

[17] R. Utama, J. Piekarewicz, Phys. Rev. C **96**, 044308 (2017).

[18] Z. M. Niu, H. Z. Liang, Phys. Lett. B **778**, 48 – 53 (2018).

[19] L. Neufcourt, Y. C. Cao, W. Nazarewicz, F. Viens, Phys. Rev.C **98**, 034318 (2018).

[20] Z. M. Niu, H. Z. Liang, B. H. Sun, Y. F. Niu,J. Y. Guo, J. Meng, Sci. Bull. **63** 759 – 764 (2018).

[21] N. N. Ma, H. F. Zhang, P. Yin, X. J. Bao, H. F. Zhang, Phys.Rev. C **96**, 024302 (2017).

[22] Z. M. Niu, B. H. Sun, H. Z. Liang, Y. F. Niu, J. Y. Guo, Phys.Rev. C **94**, 054315 (2016).

[23] X. H. Wu and P. W. Zhao, "Predicting nuclear masses with the kernel ridge regression" Phys. Rev. C **101**, 051301(R) (2020) .

[24] Z. M. Niu, J. Y. Fang, Y. F. Niu, Phys. Rev. C **100**, 054311 (2019).

[25] X.H. Wu, L.H. Guo, P.W. Zhao, Phys. Lett. B **819**, 136387 (2021).

[26] T. X. Huang, X. H. Wu and P. W. Zhao, *Commun. Theor. Phys.* **74,** 095302 (2022).

[27] X.H. Wu, Frontiers in Physics, 1-7, (2023).

[28] X.H. Wu and C. Pan, Phys. Rev. C **110**, 034322 (2024).

[29] C. F. Von Weizsäcker, Zeitschrift fürPhysik A Hadrons and Nuclei **96**, 431-458 (1935).

[30] G. Royer, B. Remaud, Nucl. Phys. vol. A444, P. 477-497(1985).

*Contact author: ajanta.das@heritageit.edu